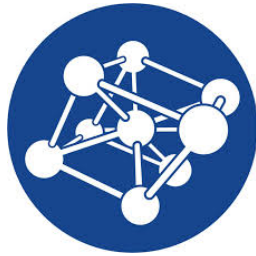




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Reactor Physics Calculations

The SP_3 -method
Analytical and numerical approaches in one dimension

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Contents

- 1 The one-dimensional P_3 -equations** **3**

- 2 The one-dimensional Marshak-type boundary condition** **5**

- 3 The three-dimensional SP_3 -equations** **7**

- 4 Marshak boundary condition for the SP_3 -equations** **10**

- 5 Solution methods of the one-dimensional SP_3 -equations** **12**
 - 5.1 Analytical solution of the one-dimensional SP_3 -equations in Cartesian coordinate system 12
 - 5.2 Numerical solution of the one-dimensional SP_3 -equations in Cartesian coordinate system using finite element method 16

1 The one-dimensional P_3 -equations

The following assumptions are made in this section:

- number of groups: G ;
- stationary state;
- geometry: one-dimensional slab;
- order of the expansion: $L = 3$.

For the one-dimensional P_L -equations, the angular flux and the scattering cross section are expanded in Legendre polynomials¹ as follows:

$$\Phi(z, E, \mu) \cong \sum_{l=0}^L \frac{2l+1}{4\pi} \Phi_l(z, E) \cdot P_l(\mu), \quad (1)$$

$$\Sigma_s(E' \rightarrow E, \mu_0) = \sum_{l=0}^{\infty} \frac{2l+1}{4\pi} \Sigma_{sl}(E' \rightarrow E) \cdot P_l(\mu_0). \quad (2)$$

For the above equations the following hold:

- the normalization applied is Y_l^0 normalized to 1;
- in one dimension, the angular flux depends only on the z coordinate and on the z component of the $\underline{\Omega}$ flying angle ($\mu = \Omega_z$ and is also the cosine of the flying angle);
- $\mu_0 = \underline{\Omega} \underline{\Omega}'$ – where $\underline{\Omega}'$ is the flying angle after scattering – is the cosine of the scattering angle.

The relation between the $P_l(\mu)$ Legendre polynomial and the $Y_l^0(\theta, \varphi)$ spherical harmonics is as follows:

$$P_l(\cos \theta) \sqrt{\frac{2l+1}{4\pi}} = Y_l^0(\theta, \varphi). \quad (3)$$

The P_l -equation is discretized over energy by applying the multi-group approximation:

$$\Phi_{l,g}(z) = \int_{E_g}^{E_{g-1}} \Phi_l(z, E) dE, \quad (4)$$

$$\int_0^{\infty} \Sigma_i(z, E) \Phi_l(z, E) dE = \sum_{g=1}^G \int_{E_g}^{E_{g-1}} \Sigma_i(z, E) \Phi_l(z, E) dE = \sum_{g=1}^G \Sigma_{i,g}(z) \Phi_{l,g}(z), \quad (5)$$

¹The name of the P_N - or also called P_L -equations comes from the $P_n(x)$ polynomial solution of the Legendre differential equation that are called Legendre polynomials. Legendre polynomials are also the simplest form of the spherical harmonics in Cartesian coordinates, where spherical harmonics can be defined as homogeneous polynomials of degree l in (x, y, z) that satisfy the Laplace equation.

$$\Sigma_{i,g}(z) = \frac{\int_{E_g}^{E_{g-1}} \Sigma_i(z, E) \Phi_l(z, E) dE}{\int_{E_g}^{E_{g-1}} \Phi_l(z, E) dE}. \quad (6)$$

Usually lower g indicates higher energy group, therefore if two-group approximation is applied $g = 1$ denotes the fast group, while $g = 2$ denotes the thermal group.

For scattering³ the group constant is generated as follows:

$$\int_{E_g}^{E_{g-1}} \left(\int_0^\infty \Sigma_{sl}(z, E' \rightarrow E) \Phi_l(z, E') dE' \right) dE = \sum_{g'=1}^G \Sigma_{sl}^{g' \rightarrow g}(z) \Phi_{lg'}(z) = \sum_{g'=1}^G \Sigma_{sl}^{g' \rightarrow g}(z) \int_{E'_g}^{E_{g'-1}} \Phi_l(z, E') dE', \quad (7)$$

$$\Sigma_{sl}^{g' \rightarrow g}(z) = \frac{\int_{E_g}^{E_{g-1}} \left(\int_{E_{g'}}^{E_{g'-1}} \Sigma_{sl}(z, E' \rightarrow E) \Phi_l(z, E') dE' \right) dE}{\int_{E_{g'}}^{E_{g'-1}} \Phi_l(z, E') dE'}, \quad (8)$$

while the group constant for the fission spectrum is generated in the following way:

$$\int_{E_g}^{E_{g-1}} f(E) \left(\int_0^\infty \nu \Sigma_f(z, E') \Phi_l(z, E') dE' \right) dE = \int_{E_g}^{E_{g-1}} f(E) \sum_{g'=1}^G \nu \Sigma_f^{g'}(z) \Phi_l^{g'}(z) dE = f_g \sum_{g'=1}^G \nu \Sigma_f^{g'}(z) \Phi_l^{g'}(z), \quad (9)$$

$$f_g = \int_{E_g}^{E_{g-1}} f(E) dE. \quad (10)$$

In the multi-group approximation, the one-dimensional P_3 -equations for the energy group g are the followings ($l = 0, \dots, 3$):

$$\frac{\partial}{\partial z} \left[\frac{l}{2l+1} \Phi_{l-1}^g(z) + \frac{l+1}{2l+1} \Phi_{l+1}^g(z) \right] + \sum_{g'=1}^G [\Sigma_g^t(z) \delta_{gg'} - \Sigma_{g' \rightarrow g}^{sl}(z)] \Phi_l^{g'}(z) = \frac{1}{k_{eff}} f_g \cdot \sum_{g'=1}^G \nu_{g'} \Sigma_{g'}^f(z) \cdot \Phi_l^{g'}(z) \cdot \delta_{l0}. \quad (11)$$

In the case of $l = 0$ $\Phi_{l-1} = 0$, similarly in the case of $l = 3$, $\Phi_{l+1} = 0$, with that the expansion is truncated at $l = 3$.

As seen above, the P_L -equations give a system of $L+1$ moment-equations with $L+2$ unknowns, but the equations are closed at $L+1$, which is straightforward in the case of static problems and does not cause any problems. In the case of time-dependent applications of the P_L -equations, this may result in a non-physical wave propagation speed.

³The scattering cross section is the sum of the cross sections for elastic and inelastic scatterings.

2 The one-dimensional Marshak-type boundary condition

In this subsection the vacuum type boundary condition is discussed, which means that there are no incoming neutrons on the boundary. In the P_L -approximation, one of the vacuum type boundary condition approximations is the Marshak boundary condition.

The generalized vacuum boundary condition can be written as:

$$\Phi^g(z, \mu_{in}) = \Phi_{bound}^g(z, \mu_{in}) = 0, \quad (12)$$

where μ_{in} is a set of direction cosines that are incident to a given boundary.

The Marshak boundary condition approximately satisfies the above equation, and it is consistent with the P_L -approximation.

The generalized Marshak-boundary condition equations are, if the boundary surface is a plane:

$$2\pi \int_{\mu_{in}} P_i(\mu) \Phi^g(x, \mu) d\mu = 0 \quad i = 1, 3, 5, \dots, L, \quad (13)$$

where $\mu = \underline{\Omega} \cdot \underline{N}_{bound}$, and \underline{N}_{bound} is the normal vector of the boundary surface element. Based on the Marshak boundary condition equations, the odd moments of the flux shall vanish on the boundary for the incoming neutron directions.

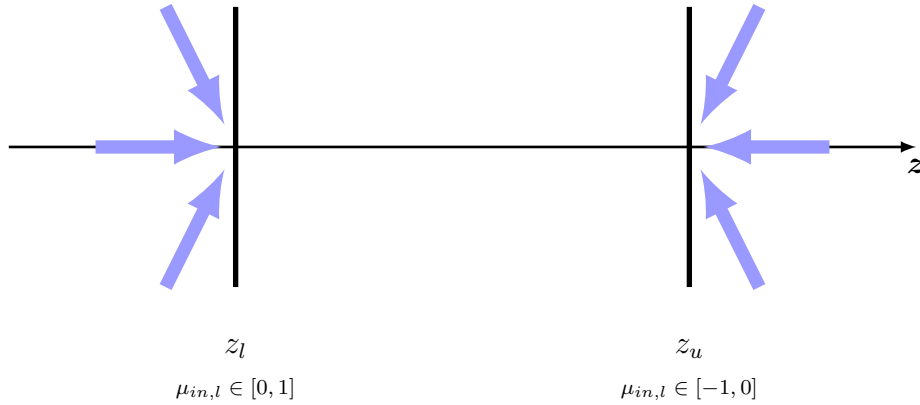


Figure 1: Incoming neutron directions at the boundaries of a one-dimensional slab

By applying the Legendre polynomial expansion also in the case of the boundary equations, we obtain the followings (if an expansion until the third moment is assumed):

$$2\pi \int_{\mu_{in}} P_i(\mu) \sum_{l=0}^L \frac{2l+1}{4\pi} \Phi_l^g(z) P_l(\mu) d\mu = 0 \quad i = 1, 3. \quad (14)$$

These equations yield $\frac{L+1}{2}$ fully coupled equations in each group and at each boundary, therefore they fully close the $L+1$ P_L -equations.

For the one-dimensional slab geometry, the boundary equations closing the one-dimensional P_3 -equations on e.g. the lower boundary (from now on the z variable is omitted for simplicity):

$$2\pi \int_0^1 P_1(\mu) \cdot \left[\frac{1}{4\pi} \Phi_0^g P_0(\mu) + \frac{3}{4\pi} \Phi_1^g P_1(\mu) + \frac{5}{4\pi} \Phi_2^g P_2(\mu) + \frac{7}{4\pi} \Phi_3^g P_3(\mu) \right] d\mu = 0, \quad (15)$$

$$2\pi \int_0^1 P_3(\mu) \cdot \left[\frac{1}{4\pi} \Phi_0^g P_0(\mu) + \frac{3}{4\pi} \Phi_1^g P_1(\mu) + \frac{5}{4\pi} \Phi_2^g P_2(\mu) + \frac{7}{4\pi} \Phi_3^g P_3(\mu) \right] d\mu = 0. \quad (16)$$

The same equations are obtained for the upper boundary, but the integration goes from -1 to 0 .

Therefore the following integrals need to be calculated:

$$\begin{aligned} \int_0^1 P_1(\mu) P_0(\mu) d\mu &= \frac{1}{2}, \\ \int_0^1 P_1(\mu) P_1(\mu) d\mu &= \frac{1}{3}, \\ \int_0^1 P_1(\mu) P_2(\mu) d\mu &= \frac{1}{8}, \\ \int_0^1 P_1 P_3 d\mu &= \int_0^1 P_3 P_1 d\mu = 0, \\ \int_0^1 P_3(\mu) P_0(\mu) d\mu &= -\frac{1}{8}, \\ \int_0^1 P_3(\mu) P_2(\mu) d\mu &= \frac{1}{8}, \\ \int_0^1 P_3(\mu) P_3(\mu) d\mu &= \frac{1}{7}, \end{aligned} \quad (17)$$

where the Legendre polynomials have the following form:

$$\begin{aligned} P_0(\mu) &= 1, \\ P_1(\mu) &= \mu, \\ P_2(\mu) &= \frac{1}{2} (3\mu^2 - 1), \\ P_3(\mu) &= \frac{1}{2} (5\mu^3 - 3\mu). \end{aligned} \quad (18)$$

The same integrations shall be performed for $\int_{-1}^0 \dots d\mu$.

After that the integrals are calculated, the following pair of equations are obtained for the lower and upper boundaries:

- for the lower boundary:

$$\begin{aligned} \frac{1}{2} \Phi_0^g + \Phi_1^g + \frac{5}{8} \Phi_2^g &= 0, \\ -\frac{1}{8} \Phi_0^g + \Phi_3^g + \frac{5}{8} \Phi_2^g &= 0, \end{aligned} \quad (19)$$

- and for the upper boundary:

$$\begin{aligned}
-\frac{1}{2} \Phi_0^g + \Phi_1^g - \frac{5}{8} \Phi_2^g &= 0, \\
\frac{1}{8} \Phi_0^g + \Phi_3^g - \frac{5}{8} \Phi_2^g &= 0.
\end{aligned} \tag{20}$$

The Marshak boundary condition equations have the same form in the SP_3 -approximation.

3 The three-dimensional SP_3 -equations

In order to get the SP_N -equations – based on Gelbard’s derivation – the following substitutions and operations are performed in the one-dimensional P_L -equations:

1. $\frac{\partial}{\partial z} \rightarrow \frac{\partial}{\partial x_i}$ and later on $\frac{\partial}{\partial x_i} \rightarrow \nabla$ (gradient or divergence);
2. the odd flux moments are expressed by using the odd moment equations;
3. the odd flux moments are eliminated from the even moment equations.

With the above procedure, such a system of moment equations is obtained that has half the size of the P_L -equations, and the number of unknowns are also reduced to half. The obtained equations, where the flux moments are space-dependent:

$$-l = 0:$$

$$\frac{\partial}{\partial x_i} [\Phi_1^g] + \sum_{g'=1}^G [\Sigma_g^t \delta_{gg'} - \Sigma_{g' \rightarrow g}^{s0}] \Phi_0^{g'} = \frac{1}{k_{eff}} f_g \sum_{g'=1}^G \nu_{g'} \Sigma_{g'}^f \Phi_0^{g'}, \tag{21}$$

$$-l = 1:$$

$$\frac{\partial}{\partial x_i} \left[\frac{1}{3} \Phi_0^g + \frac{2}{3} \Phi_2^g \right] + \sum_{g'=1}^G [\Sigma_g^t \delta_{gg'} - \Sigma_{g' \rightarrow g}^{s1}] \Phi_1^{g'} = 0, \tag{22}$$

$$-l = 2:$$

$$\frac{\partial}{\partial x_i} \left[\frac{2}{5} \Phi_1^g + \frac{3}{5} \Phi_2^g \right] + \sum_{g'=1}^G [\Sigma_g^t \delta_{gg'} - \Sigma_{g' \rightarrow g}^{s2}] \Phi_2^{g'} = 0, \tag{23}$$

$$-l = 3:$$

$$\frac{\partial}{\partial x_i} \left[\frac{3}{7} \Phi_2^g \right] + \sum_{g'=1}^G [\Sigma_g^t \delta_{gg'} - \Sigma_{g' \rightarrow g}^{s3}] \Phi_3^{g'} = 0. \tag{24}$$

Let’s consider G energy group, and introduce the following vector and matrix notations:

$$\underline{\Phi}_l = \begin{bmatrix} \Phi_l^1 \\ \Phi_l^2 \\ \vdots \\ \Phi_l^G \end{bmatrix}, \tag{25}$$

$$\underline{\underline{\Sigma}}_l = \begin{bmatrix} \Sigma_1^t - \Sigma_{11}^{sl} & -\Sigma_{21}^{sl} & \cdots & -\Sigma_{G1}^{sl} \\ -\Sigma_{12}^{sl} & \Sigma_2^t - \Sigma_{22}^{sl} & \cdots & -\Sigma_{G2}^{sl} \\ \vdots & \vdots & \ddots & \vdots \\ -\Sigma_{1G}^{sl} & -\Sigma_{2G}^{sl} & \cdots & \Sigma_G^t - \Sigma_{GG}^{sl} \end{bmatrix}, \quad (26)$$

and

$$\underline{\underline{\Sigma}}_F = \begin{bmatrix} f_1 \nu_1 \Sigma_1^f & f_1 \nu_2 \Sigma_2^f & \cdots & f_1 \nu_G \Sigma_G^f \\ f_2 \nu_1 \Sigma_1^f & f_2 \nu_2 \Sigma_2^f & \cdots & f_2 \nu_G \Sigma_G^f \\ \vdots & \vdots & \ddots & \vdots \\ f_G \nu_1 \Sigma_1^f & f_G \nu_2 \Sigma_2^f & \cdots & f_G \nu_G \Sigma_G^f \end{bmatrix}. \quad (27)$$

With these notations, the following matrix equations are obtained:

- $l = 0$:

$$\frac{\partial}{\partial x_i} \Phi_1 + \underline{\underline{\Sigma}}_0 \cdot \Phi_0 = \frac{1}{k_{eff}} \cdot \underline{\underline{\Sigma}}_F \cdot \Phi_0, \quad (28)$$

- $l = 1$:

$$\frac{\partial}{\partial x_i} \left[\frac{1}{3} \Phi_0 + \frac{2}{3} \Phi_2 \right] + \underline{\underline{\Sigma}}_1 \cdot \Phi_1 = 0, \quad (29)$$

- $l = 2$:

$$\frac{\partial}{\partial x_i} \left[\frac{2}{5} \Phi_1 + \frac{3}{5} \Phi_3 \right] + \underline{\underline{\Sigma}}_2 \cdot \Phi_2 = 0, \quad (30)$$

- $l = 3$:

$$\frac{\partial}{\partial x_i} \left[\frac{3}{7} \Phi_2 \right] + \underline{\underline{\Sigma}}_3 \cdot \Phi_3 = 0. \quad (31)$$

From the moment equations $l = 1$ and $l = 3$, Φ_1 and Φ_3 are expressed as follows:

$$\Phi_3 = -\underline{\underline{\Sigma}}_3^{-1} \frac{\partial}{\partial x_i} \left[\frac{3}{7} \Phi_2 \right], \quad (32)$$

$$\Phi_1 = -\underline{\underline{\Sigma}}_1^{-1} \frac{\partial}{\partial x_i} \left[\frac{1}{3} \Phi_0 + \frac{2}{3} \Phi_2 \right], \quad (33)$$

that are substituted back to the $l = 0$ and $l = 2$ moment equations:

- $l = 0$:

$$-\frac{\partial}{\partial x_i} \underline{\underline{\Sigma}}_1^{-1} \frac{\partial}{\partial x_i} \left[\frac{1}{3} \Phi_0 + \frac{2}{3} \Phi_2 \right] + \underline{\underline{\Sigma}}_0 \cdot \Phi_0 = \frac{1}{k_{eff}} \cdot \underline{\underline{\Sigma}}_F \cdot \Phi_0, \quad (34)$$

- $l = 2$:

$$-\frac{\partial}{\partial x_i} \left[\frac{2}{5} \underline{\underline{\Sigma}}_1^{-1} \frac{\partial}{\partial x_i} \left[\frac{1}{3} \Phi_0 + \frac{2}{3} \Phi_2 \right] + \frac{3}{5} \underline{\underline{\Sigma}}_3^{-1} \frac{\partial}{\partial x_i} \left[\frac{3}{7} \Phi_2 \right] \right] + \underline{\underline{\Sigma}}_2 \cdot \Phi_2 = 0. \quad (35)$$

The following new variables are introduced:

$$\underline{U}_1 := \underline{\Phi}_0 + 2 \underline{\Phi}_2 \quad \rightarrow \quad \underline{\Phi}_0 = \underline{U}_1 - \frac{2}{3} \underline{U}_2, \quad (36)$$

$$\underline{U}_2 := 3 \underline{\Phi}_2 \quad \rightarrow \quad \underline{\Phi}_2 = \frac{1}{3} \underline{U}_2. \quad (37)$$

With the new variables the following equations are obtained:

- $l = 0$:

$$-\frac{1}{3} \frac{\partial}{\partial x_i} \underline{\Sigma}_1^{-1} \frac{\partial}{\partial x_i} \underline{U}_1 + \underline{\Sigma}_0 \cdot \left(\underline{U}_1 - \frac{2}{3} \underline{U}_2 \right) = \frac{1}{k_{eff}} \cdot \underline{\Sigma}_F \cdot \left(\underline{U}_1 - \frac{2}{3} \underline{U}_2 \right), \quad (38)$$

- $l = 2$:

$$-\frac{\partial}{\partial x_i} \left[\frac{2}{15} \underline{\Sigma}_1^{-1} \frac{\partial}{\partial x_i} \underline{U}_1 + \frac{3}{35} \underline{\Sigma}_3^{-1} \frac{\partial}{\partial x_i} \underline{U}_2 \right] + \frac{1}{3} \underline{\Sigma}_2 \cdot \underline{U}_2 = 0. \quad (39)$$

Effective diffusion coefficients can be introduced based on the following definitions:

$$\underline{D}_1 = \frac{1}{3} \underline{\Sigma}_1^{-1}, \quad (40)$$

$$\underline{D}_3 = \frac{1}{7} \underline{\Sigma}_3^{-1}, \quad (41)$$

which yield the moment equations:

- $l = 0$:

$$-\frac{\partial}{\partial x_i} \underline{D}_1 \frac{\partial}{\partial x_i} \underline{U}_1 + \underline{\Sigma}_0 \cdot \left(\underline{U}_1 - \frac{2}{3} \underline{U}_2 \right) = \frac{1}{k_{eff}} \cdot \underline{\Sigma}_F \cdot \left(\underline{U}_1 - \frac{2}{3} \underline{U}_2 \right), \quad (42)$$

- $l = 2$:

$$-\frac{\partial}{\partial x_i} \left[\frac{2}{5} \underline{D}_1 \frac{\partial}{\partial x_i} \underline{U}_1 + \frac{3}{5} \underline{D}_3 \frac{\partial}{\partial x_i} \underline{U}_2 \right] + \frac{1}{3} \underline{\Sigma}_2 \cdot \underline{U}_2 = 0. \quad (43)$$

From the moment equation $l = 0$:

$$-\frac{\partial}{\partial x_i} \underline{D}_1 \frac{\partial}{\partial x_i} \underline{U}_1 = -\underline{\Sigma}_0 \cdot \left(\underline{U}_1 - \frac{2}{3} \underline{U}_2 \right) + \frac{1}{k_{eff}} \cdot \underline{\Sigma}_F \cdot \left(\underline{U}_1 - \frac{2}{3} \underline{U}_2 \right), \quad (44)$$

which can be substituted back to the moment equation $l = 2$:

$$-\frac{2}{5} \underline{\Sigma}_0 \cdot \left(\underline{U}_1 - \frac{2}{3} \underline{U}_2 \right) + \frac{2}{5} \frac{1}{k_{eff}} \cdot \underline{\Sigma}_F \cdot \left(\underline{U}_1 - \frac{2}{3} \underline{U}_2 \right) - \frac{\partial}{\partial x_i} \left(\frac{3}{5} \underline{D}_3 \frac{\partial}{\partial x_i} \underline{U}_2 \right) + \frac{1}{3} \underline{\Sigma}_2 \cdot \underline{U}_2 = 0. \quad (45)$$

By multiplying the moment equation $l = 2$ by $\frac{5}{3}$, the final form of the one-dimensional SP_3 -equations is obtained:

- $l = 0$:

$$-\frac{\partial}{\partial x_i} \underline{D}_1 \frac{\partial}{\partial x_i} U_1 + \underline{\Sigma}_0 \cdot \left(U_1 - \frac{2}{3} U_2 \right) = \frac{1}{k_{eff}} \cdot \underline{\Sigma}_F \cdot \left(U_1 - \frac{2}{3} U_2 \right), \quad (46)$$

- $l = 2$:

$$-\frac{\partial}{\partial x_i} \underline{D}_3 \frac{\partial}{\partial x_i} U_2 - \frac{2}{3} \underline{\Sigma}_0 \cdot U_1 + \left(\frac{4}{9} \underline{\Sigma}_0 + \frac{5}{9} \underline{\Sigma}_2 \right) U_2 = -\frac{1}{k_{eff}} \cdot \frac{2}{3} \cdot \underline{\Sigma}_F \cdot \left(U_1 - \frac{2}{3} U_2 \right). \quad (47)$$

According to Gelbard's derivation the three-dimensional equations can be obtained as follows:

$$-\nabla \underline{D}_1 \nabla U_1 + \underline{\Sigma}_0 \cdot \left(U_1 - \frac{2}{3} U_2 \right) = \frac{1}{k_{eff}} \cdot \underline{\Sigma}_F \cdot \left(U_1 - \frac{2}{3} U_2 \right), \quad (48)$$

$$-\nabla \underline{D}_3 \nabla U_2 - \frac{2}{3} \underline{\Sigma}_0 \cdot U_1 + \left(\frac{4}{9} \underline{\Sigma}_0 + \frac{5}{9} \underline{\Sigma}_2 \right) U_2 = -\frac{1}{k_{eff}} \cdot \frac{2}{3} \underline{\Sigma}_F \cdot \left(U_1 - \frac{2}{3} U_2 \right). \quad (49)$$

With this method $\frac{L+1}{2}$ moment equations are obtained with $\frac{L+1}{2}$ variables. These are a series of elliptic, second-order differential equations, each of them having a diffusion-like form.

4 Marshak boundary condition for the SP_3 -equations

Using the vector notations in the case of the boundary equations, the followings are obtained for the upper and lower boundaries:

$$\mp \frac{1}{2} \Phi_0 + \Phi_1 \mp \frac{5}{8} \Phi_2 = 0, \quad (50)$$

$$\pm \frac{1}{8} \Phi_0 + \Phi_3 \mp \frac{5}{8} \Phi_2 = 0. \quad (51)$$

Based on the previous subsection – by performing the similar substitutions – the following equations are obtained:

$$\mp \frac{1}{2} \Phi_0 - \underline{\Sigma}_1^{-1} \frac{\partial}{\partial x_i} \left[\frac{1}{3} \Phi_0 + \frac{2}{3} \Phi_2 \right] \mp \frac{5}{8} \Phi_2 = 0, \quad (52)$$

$$\pm \frac{1}{8} \Phi_0 - \underline{\Sigma}_3^{-1} \frac{\partial}{\partial x_i} \left[\frac{3}{7} \Phi_2 \right] \mp \frac{5}{8} \Phi_2 = 0. \quad (53)$$

By applying the new variables U_1 and U_2 , as well as the \underline{D}_1 and \underline{D}_3 effective diffusion coefficients, and also introducing the $\frac{\partial}{\partial x_i} \rightarrow \nabla$ (gradient) substitution, the Marshak boundary condition equations will have the following form:

$$-\underline{D}_1 \nabla U_1 \mp \frac{1}{2} U_1 \pm \frac{1}{8} U_2 = 0, \quad (54)$$

$$-\underline{D}_3 \nabla U_2 \pm \frac{1}{8} U_1 \mp \frac{7}{24} U_2 = 0. \quad (55)$$

In the SP_3 Marshak boundary condition, equations the flux moments are coupled on the boundary. Based on these equations, effective currents can also be defined as \underline{J}_1 and \underline{J}_2 by applying Fick's law as follows:

$$\underline{J}_1 = -\underline{D}_1 \nabla \underline{U}_1, \quad (56)$$

$$\underline{J}_2 = -\underline{D}_3 \nabla \underline{U}_2. \quad (57)$$

In the case of reflective boundary condition the effective currents yield zero on the boundaries, i.e. $\underline{J}_1 = 0$ and $\underline{J}_2 = 0$, therefore $\nabla \underline{U}_1 = 0$ and $\nabla \underline{U}_2 = 0$.

Summary:

In the previous part of the lecture, the SP_3 -equations were derived that yield two second-order, elliptic, diffusion-like differential equations. The SP_3 Marshak boundary condition equations were also given in the case of vacuum boundaries, as well as the equations for the zero effective current in the case of reflective boundaries. Each boundary condition type yields two first-order, (Robin-type) conditions that closes the system of SP_3 -equations.

5 Solution methods of the one-dimensional SP_3 -equations

5.1 Analytical solution of the one-dimensional SP_3 -equations in Cartesian coordinate system

In this subsection the following assumptions are made:

- geometry: one-dimensional, symmetric slab (Cartesian geometry);
- material composition: homogeneous, containing homogenized fissile material;
- boundaries: vacuum boundary condition;
- stationary-state;
- number of groups: one energy group.

With the above assumptions the \underline{U}_1 and \underline{U}_2 vectors become scalar $\rightarrow U_1$ and U_2 , while the group constants are as follows:

$$\underline{\underline{\Sigma}}_l = \Sigma^t - \Sigma_{11}^{sl} := \Sigma^{Rl}, \quad (58)$$

$$\underline{\underline{\Sigma}}_F = \nu \Sigma^f, \quad (59)$$

$$\underline{\underline{D}}_1 = \frac{1}{3 \Sigma^{R1}} := D_1, \quad (60)$$

$$\underline{\underline{D}}_3 = \frac{1}{7 \Sigma^{R3}} := D_3. \quad (61)$$

In the analysed case the SP_3 -equations have the following form:

- $l = 0$:

$$- D_1 \Delta U_1 + \Sigma^{R0} \left(U_1 - \frac{2}{3} U_2 \right) = \frac{1}{k_{eff}} \nu \Sigma^f \left(U_1 - \frac{2}{3} U_2 \right), \quad (62)$$

- $l = 2$:

$$- D_3 \Delta U_2 - \frac{2}{3} \Sigma^{R0} U_1 + \left(\frac{4}{9} \Sigma^{R0} + \frac{5}{9} \Sigma^{R2} \right) U_2 = - \frac{1}{k_{eff}} \frac{2}{3} \nu \Sigma^f \left(U_1 - \frac{2}{3} U_2 \right). \quad (63)$$

The matrix form of the above equation system is:

$$\begin{bmatrix} -D_1 \Delta + \Sigma^{R0} - \frac{1}{k_{eff}} \nu \Sigma^f & -\frac{2}{3} \Sigma^{R0} + \frac{2}{3} \frac{1}{k_{eff}} \nu \Sigma^f \\ -\frac{2}{3} \Sigma^{R0} + \frac{2}{3} \frac{1}{k_{eff}} \nu \Sigma^f & -D_3 \Delta + \frac{4}{9} \Sigma^{R0} + \frac{5}{9} \Sigma^{R2} - \frac{4}{9} \frac{1}{k_{eff}} \nu \Sigma^f \end{bmatrix} \cdot \begin{bmatrix} U_1 \\ U_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}. \quad (64)$$

The mathematical form of these equations is similar to the two-group diffusion equations where the group fluxes satisfy the Helmholtz equation as follows:

$$\Delta \Phi^g(x) + B^2 \Phi^g(x) = 0 \quad g \in 1, \dots, G . \quad (65)$$

Here the similar equation holds for U_1 and U_2 :

$$\Delta U_i(x) + B^2 U_i(x) = 0 \quad i = 1, 2 . \quad (66)$$

Therefore the Laplace-operator can be substituted by its eigenvalue $-B^2$:

$$\begin{bmatrix} D_1 B^2 + \Sigma^{R0} - \frac{1}{k_{eff}} \nu \Sigma^f & -\frac{2}{3} \Sigma^{R0} + \frac{2}{3} \frac{1}{k_{eff}} \nu \Sigma^f \\ -\frac{2}{3} \Sigma^{R0} + \frac{2}{3} \frac{1}{k_{eff}} \nu \Sigma^f & D_3 B^2 + \frac{4}{9} \Sigma^{R0} + \frac{5}{9} \Sigma^{R2} - \frac{4}{9} \frac{1}{k_{eff}} \nu \Sigma^f \end{bmatrix} \cdot \begin{bmatrix} U_1 \\ U_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} . \quad (67)$$

In order to simplify the derivation of the solution, let us introduce the following notations:

$$a := \Sigma^{R0} - \frac{1}{k_{eff}} \nu \Sigma^f, \quad (68)$$

$$b := \frac{4}{9} a + \frac{5}{9} \Sigma^{R2}. \quad (69)$$

With the above notations the matrix equation will have the following form:

$$\begin{bmatrix} D_1 B^2 + a & -\frac{2}{3} a \\ -\frac{2}{3} a & D_3 B^2 + b \end{bmatrix} \cdot \begin{bmatrix} U_1 \\ U_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} . \quad (70)$$

In order to yield a non-trivial solution – being a homogeneous, linear differential equation system – the determinant of the matrix coefficient in the above matrix equation has to be zero according to the following equation:

$$\det \underline{\underline{M}} = (D_1 B^2 + a) (D_3 B^2 + b) - \frac{4}{9} a^2 = 0. \quad (71)$$

This equation gives us the relation between the geometry, boundary conditions, material properties and the effective multiplication factor.

From the above equation k_{eff} can be expressed in the following form:

$$k_{eff} = \frac{\nu \Sigma^f \left[\left(\frac{4}{9} D_1 + D_3 \right) B^2 + \frac{5}{9} \Sigma^{R2} \right]}{D_1 D_3 B^4 + \left[D_1 \left(\frac{4}{9} \Sigma^{R0} + \frac{5}{9} \Sigma^{R2} \right) + D_3 \Sigma^{R0} \right] B^2 + \frac{5}{9} \Sigma^{R0} \Sigma^{R2}}, \quad (72)$$

while the buckling parameters are:

$$B_{1,2}^2 = \frac{-(a D_3 + b D_1) \pm \sqrt{(a D_3 + b D_1)^2 - 4 D_1 D_3 (a b - \frac{4}{9} a^2)}}{2 D_1 D_3}. \quad (73)$$

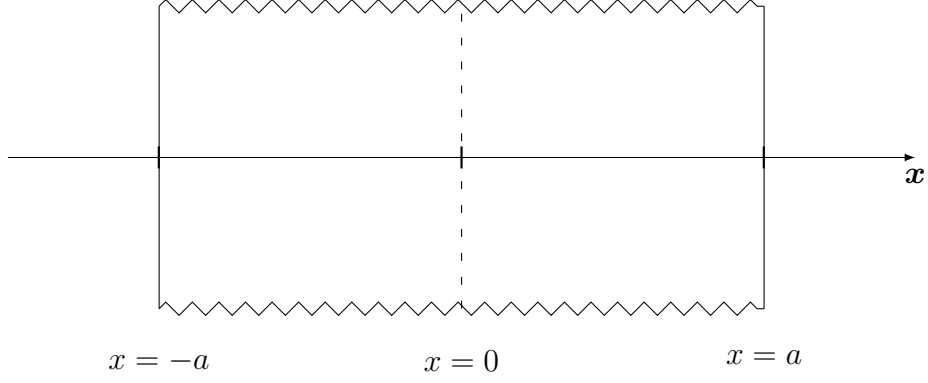


Figure 2: One-dimensional, symmetric slab geometry

In the case of one-dimensional slab geometry, by applying symmetry considerations and having $x = 0$ at the half-width of the geometry, the solution of the matrix equation will be

$$U_2 = A_1 \cos(B_1 x) + A_2 \cos(B_2 x), \quad (74)$$

while – because the flux moments are coupled in the differential equation system – the form of U_1 will be:

$$U_1 = \frac{3}{2a} (D_3 B_1^2 + b) A_1 \cos(B_1 x) + \frac{3}{2a} (D_3 B_2^2 + b) A_2 \cos(B_2 x). \quad (75)$$

By introducing the following notations, again for simplification purposes:

$$c := \frac{3}{2a} (D_3 B_1^2 + b), \quad (76)$$

$$d := \frac{3}{2a} (D_3 B_2^2 + b), \quad (77)$$

the solution function for U_1 will have the following form:

$$U_1 = c A_1 \cos(B_1 x) + d A_2 \cos(B_2 x). \quad (78)$$

To determine A_1 and A_2 , boundary condition equations are needed. In the case of vacuum boundaries, the Marshak boundary condition equations:

- for the lower boundary:

$$\frac{1}{2} U_1(x = -a) - \frac{1}{8} U_2(x = -a) = D_1 \frac{d}{dx} U_1|_{x=-a}, \quad (79)$$

$$-\frac{1}{8} U_1(x = -a) + \frac{7}{24} U_2(x = -a) = D_3 \frac{d}{dx} U_2|_{x=-a}, \quad (80)$$

- while for the upper boundary:

$$-\frac{1}{2} U_1(x = a) + \frac{1}{8} U_2(x = a) = D_1 \frac{d}{dx} U_1|_{x=a}, \quad (81)$$

$$\frac{1}{8} U_1(x = a) - \frac{7}{24} U_2(x = a) = D_3 \frac{d}{dx} U_2|_{x=a}. \quad (82)$$

However – because symmetry is assumed, and only two free parameters are missing – the upper boundary condition set is not needed.

The two missing parameters, A_1 and A_2 can be determined from the above equation system, by substituting back the solutions obtained for U_1 and U_2 .

Because of the arbitrary normalization of the solution of the Helmholtz equation, one of the parameters can be fixed, i. e. let A_1 equal to 1. By fixing the value of A_1 , A_2 can be determined.

The solution procedure for A_2 yields a transcendent equation system⁴, which can be solved by e.g. iteration.

⁴One equation comes from the $k_{eff} - B^2$ relation, two from the relation obtained for B^2 , while another equation is obtained from the above boundary fitting, that yield altogether four equations for A_2 , B_1 , B_2 and k_{eff} to solve iteratively.

5.2 Numerical solution of the one-dimensional SP₃-equations in Cartesian coordinate system using finite element method

This subsection provides a brief – problem-oriented – introduction into finite element discretization, which is followed by the finite element solution of the one-dimensional SP₃-equations in slab geometry.

The finite element solution of a problem usually starts with the subdivision of the analysed domain Ω into elements which are a collection of geometrically simple forms. This geometrical partition is called a mesh, while the connecting parts of the elements are called nodes and edges.

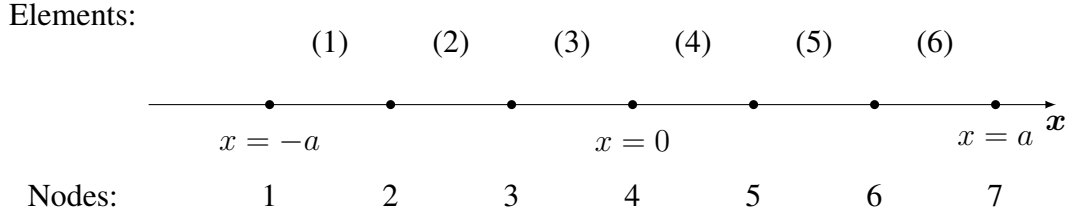


Figure 3: A simple mesh for a one-dimensional slab geometry

The number of elements within the mesh determines the characteristic length of the spatial discretization, as well as provides information about the element size. The approximate solution of the problem will be composed of piecewise polynomial functions on each element. In this subsection continuous finite element method is applied which requires that the variables at each connecting node are continuous.

After the subdivision of the one-dimensional slab geometry into elements (aka after meshing), the solution within one element is approximated – in this case – by linear interpolation of the nodal variables.

The linear interpolation within each element means that the solution functions are approximated within the elements as follows (the first index is the local nodal index, while the second stands for the moment):

$$U_1(x) \approx h_1(x) \cdot \hat{U}_{1,1} + h_2(x) \cdot \hat{U}_{2,1}, \quad (83)$$

$$U_2(x) \approx h_1(x) \cdot \hat{U}_{1,2} + h_2(x) \cdot \hat{U}_{2,2}. \quad (84)$$

The $h_i(x)$ functions are called shape functions or interpolation functions, and have the following form:

$$h_1(x) = \frac{x_2 - x}{x_2 - x_1}, \quad (85)$$

$$h_2(x) = \frac{x - x_1}{x_2 - x_1}. \quad (86)$$

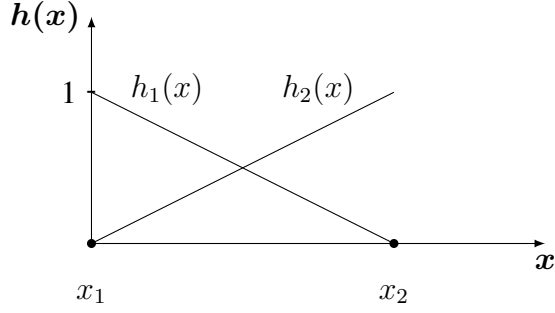


Figure 4: Linear interpolation functions in the case of the applied one-dimensional mesh

The second step of the finite element solution is the derivation of the finite element equations. By applying the matrix and vector notations of the previous subsection, the SP_3 -equations have the following form:

$$\underline{\underline{M}} \begin{bmatrix} U_1 \\ U_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}. \quad (87)$$

The variational formulation of this equation system – by introducing the trial functions V_1, V_2 – is the following:

$$\int_{\Omega} [V_1 \ V_2] \underline{\underline{M}} \begin{bmatrix} U_1 \\ U_2 \end{bmatrix} dx = 0. \quad (88)$$

The above problem – also called the weak formulation – can be defined as: find U_1 and U_2 for which the above equation holds for arbitrary V_1 and V_2 trial functions.

By using the so-called Galerkin-method, the above mathematical model equations are discretized in order to obtain the numerical model equations. The discretization implies that an approximate solution is to be found at the nodes that – due to the interpolation – leads to an internal approximation within the elements. The variational formulation for the internal approximation can be written as:

$$\int_{\Omega} [\hat{V}_1 \ \hat{V}_2] \underline{\underline{M}} \begin{bmatrix} \hat{U}_1 \\ \hat{U}_2 \end{bmatrix} dx = 0. \quad (89)$$

The approximate solution, along with the trial functions are linearly interpolated within each element as follows:

$$\begin{bmatrix} \hat{U}_1 \\ \hat{U}_2 \end{bmatrix} = \begin{bmatrix} h_1 & 0 & h_2 & 0 \\ 0 & h_1 & 0 & h_2 \end{bmatrix} \begin{bmatrix} \hat{U}_{1,1} \\ \hat{U}_{1,2} \\ \hat{U}_{2,1} \\ \hat{U}_{2,2} \end{bmatrix}, \quad (90)$$

while

$$[\hat{V}_1 \ \hat{V}_2] = [\hat{V}_{1,1} \ \hat{V}_{1,2} \ \hat{V}_{2,1} \ \hat{V}_{2,2}] \begin{bmatrix} h_1 & 0 \\ 0 & h_1 \\ h_2 & 0 \\ 0 & h_2 \end{bmatrix}. \quad (91)$$

By substituting back the above approximations – that are extended to the global system – to the variational formulation of the internal approximation, the problem definition becomes the following: find $\hat{\underline{U}}$ global variable vector such that

$$\int_{\Omega} \hat{\underline{V}}^T \underline{h}^T \underline{M} \underline{h} \hat{\underline{U}} dx = 0 \quad (92)$$

for arbitrary $\hat{\underline{V}}$ global approximate trial vector, where \underline{h} denotes the global interpolation operator.

As $\hat{\underline{U}}$ contains the approximate solution at each node, and the above equation has to hold for arbitrary trial functions, the problem can be defined as follows: find $\hat{U}_1, \hat{U}_2, \dots, \hat{U}_N$ (N denotes the number of nodes) such that:

$$\int_{\Omega} \underline{h}^T \underline{M} \underline{h} dx \hat{\underline{U}} = 0, \quad (93)$$

which formulation is therefore equivalent of solving a linear equation system such that:

$$\underline{\mathring{M}} \hat{\underline{U}} = 0. \quad (94)$$

Since the interpolation functions have a small support, most of the coefficients within the $\underline{\mathring{M}}$ global matrix coefficient are zeros. The global matrix can be obtained from assembling the element matrices that depend only on the parameters within one element, and can be evaluated by e.g. numerical integration over an element in the local coordinate system. During assembling, the contribution of the element matrices is added to the right coefficient within the global matrix.

The final step of the finite element method is the numerical solution of the above presented linear equation system that is the most computationally expensive part of the procedure.

In the case of the present problem, after meshing the one-dimensional slab geometry, e.g. by applying an equidistant grid, the numerical model equations are obtained as follows:

$$\int_{\Omega} \underline{h}^T \begin{bmatrix} -D_1 \Delta + \Sigma^{R0} - \frac{1}{k_{eff}} \nu \Sigma^f & -\frac{2}{3} \Sigma^{R0} + \frac{2}{3} \frac{1}{k_{eff}} \nu \Sigma^f \\ -\frac{2}{3} \Sigma^{R0} + \frac{2}{3} \frac{1}{k_{eff}} \nu \Sigma^f & -D_3 \Delta + \frac{4}{9} \Sigma^{R0} + \frac{5}{9} \Sigma^{R2} - \frac{4}{9} \frac{1}{k_{eff}} \nu \Sigma^f \end{bmatrix} \underline{h} dx \hat{\underline{U}} = 0. \quad (95)$$

Each term of the above equation can be rewritten in the following manner:

- the diffusion term, where – due to the one-dimensional problem – $\Delta = \frac{d^2}{dx^2}$:

$$\begin{aligned} \int_{\Omega} \underline{h}^T \begin{bmatrix} -D_1 \frac{d^2}{dx^2} & 0 \\ 0 & -D_3 \frac{d^2}{dx^2} \end{bmatrix} \underline{h} dx \cdot \hat{\underline{U}} = \\ \int_{\Omega} \frac{d}{dx} \underline{h}^T \begin{bmatrix} D_1 & 0 \\ 0 & D_3 \end{bmatrix} \frac{d}{dx} \underline{h} dx \hat{\underline{U}} - \left[\underline{h}^T \begin{bmatrix} D_1 & 0 \\ 0 & D_3 \end{bmatrix} \frac{d}{dx} \underline{h} \cdot \hat{\underline{U}} \right]_{x_1}^{x_N} = \\ = \underline{\mathring{K}} \hat{\underline{U}} - \underline{\mathring{P}}, \end{aligned} \quad (96)$$

- the scattering and absorption term is the following:

$$\int_{\Omega} \underline{h}^T \begin{bmatrix} \Sigma^{R0} & -\frac{2}{3} \Sigma^{R0} \\ -\frac{2}{3} \Sigma^{R0} & \frac{4}{9} \Sigma^{R0} + \frac{5}{9} \Sigma^{R2} \end{bmatrix} \underline{h} dx \cdot \hat{\underline{U}} = \underline{\mathring{R}} \hat{\underline{U}}, \quad (97)$$

- while the fission term is

$$\int_{\Omega} \underline{h}^T \begin{bmatrix} -\frac{1}{k_{eff}} \nu \Sigma^f & \frac{2}{3} \frac{1}{k_{eff}} \nu \Sigma^f \\ \frac{2}{3} \frac{1}{k_{eff}} \nu \Sigma^f & -\frac{4}{9} \frac{1}{k_{eff}} \nu \Sigma^f \end{bmatrix} \underline{h} dx \cdot \hat{U} = -\frac{1}{k_{eff}} \underline{\dot{X}} \hat{U}. \quad (98)$$

The obtained equation system is

$$\underline{\dot{K}} \hat{U} - \underline{\dot{P}} + \underline{\dot{R}} \hat{U} = \frac{1}{k_{eff}} \underline{\dot{X}} \hat{U}. \quad (99)$$

In order to determine the $\underline{\dot{P}}$ boundary term, the Marshak boundary condition equations are needed at the lower ($x = x_1$) and at the upper ($x = x_N$) boundaries:

$$\begin{bmatrix} \frac{1}{2} & -\frac{1}{8} \\ -\frac{1}{8} & \frac{7}{24} \end{bmatrix} \begin{bmatrix} U_1 \\ U_2 \end{bmatrix} = \begin{bmatrix} \mp D_1 \frac{dU_1}{dx} \\ \mp D_3 \frac{dU_2}{dx} \end{bmatrix}, \quad (100)$$

where the similar approximation needs to be performed as described previously within this subsection.

The boundary equations for the approximated solution are:

$$\begin{bmatrix} \frac{1}{2} & -\frac{1}{8} \\ -\frac{1}{8} & \frac{7}{24} \end{bmatrix} \underline{h} \cdot \hat{U} = \begin{bmatrix} \mp D_1 & 0 \\ 0 & \mp D_3 \end{bmatrix} \frac{d}{dx} \underline{h} \cdot \hat{U}, \quad (101)$$

based on which a substitution can be performed in the linear equation system as follows:

$$\begin{aligned} & - \left[\underline{h}^T \begin{bmatrix} D_1 & 0 \\ 0 & D_3 \end{bmatrix} \frac{d}{dx} \underline{h} \cdot \hat{U} \right]_{x_1}^{x_N} = \\ & - \left[\underline{h}^T \begin{bmatrix} D_1 & 0 \\ 0 & D_3 \end{bmatrix} \frac{d}{dx} \underline{h} \cdot \hat{U} \right]^{x_N} + \left[\underline{h}^T \begin{bmatrix} D_1 & 0 \\ 0 & D_3 \end{bmatrix} \frac{d}{dx} \underline{h} \cdot \hat{U} \right]^{x_1} = \\ & \left[\underline{h}^T \begin{bmatrix} \frac{1}{2} & -\frac{1}{8} \\ -\frac{1}{8} & \frac{7}{24} \end{bmatrix} \underline{h} \cdot \hat{U} \right]^{x_N} + \left[\underline{h}^T \begin{bmatrix} \frac{1}{2} & -\frac{1}{8} \\ -\frac{1}{8} & \frac{7}{24} \end{bmatrix} \underline{h} \cdot \hat{U} \right]^{x_1} = \\ & \left[\underline{h}^T \begin{bmatrix} \frac{1}{2} & -\frac{1}{8} \\ -\frac{1}{8} & \frac{7}{24} \end{bmatrix} \underline{h} \right]^{x_N} \cdot \hat{U} + \left[\underline{h}^T \begin{bmatrix} \frac{1}{2} & -\frac{1}{8} \\ -\frac{1}{8} & \frac{7}{24} \end{bmatrix} \underline{h} \right]^{x_1} \cdot \hat{U} = \underline{\dot{B}} \cdot \hat{U}. \end{aligned} \quad (102)$$

By evaluating the matrix terms for each elements and after an assembling procedure, the following global equation system is obtained that can be solved by a selected numerical method:

$$\underline{\dot{K}} \hat{U} + \underline{\dot{B}} \cdot \hat{U} + \underline{\dot{R}} \hat{U} = \frac{1}{k_{eff}} \underline{\dot{X}} \hat{U}, \quad (103)$$

that is

$$\underline{\dot{A}} \hat{U} = \frac{1}{k_{eff}} \underline{\dot{X}} \hat{U}. \quad (104)$$